An Equation of State for Opacity Calculations

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In this paper we report on CHEMEOS, the new equation of state (EOS) model developed for the new Los Alamos National Laboratory low-to-medium-Z-element opacity code ATOMIC. ATOMIC is used to produce plasma opacity tables that are needed to describe the transport of energy by radiation in plasma hydrodynamics simulations. An EOS model is a first step in generating opacity data in which the populations of various atomic species in a plasma of a given temperature and density are calculated. These populations are then postprocessed in ATOMIC to yield spectral properties, which finally translate into plasma opacity data.

Our EOS model provides local-thermal-equilibrium (LTE) ion stage populations calculated with a thermodynamically consistent account of nonideal plasma effects, which disallow the simple description of the plasma as an ideal gas. To this end we have followed a free-energy-minimization approach [1] in deriving the ion population equations for the thermodynamic equilibrium EOS for ATOMIC. The resulting equations can be formulated to resemble modified Saha-type equations with guaranteed thermodynamic consistency since all population and thermodynamic quantities are derived from a single expression for the total Helmholtz free energy $F(V,T,\{N_s\})$ for the entire system [2-5]. The solution of the system of Saha-type equations is the collection of populations $\{N_s\}_{min}$ which minimizes the free energy at a given temperature and mass density. The formal procedure also satisfies the stoichiometric constraints for ionization or molecular dissociation, as well as overall plasma charge neutrality and mass conservation conditions.

Inherent in this formalism is the use of the chemical picture in which the plasma constituents are viewed as atoms, molecules, ions, and free electrons. Our choice of the chemical picture is largely due to its theoretical transparency and adaptability to the large range of physical conditions required in opacity calculations.

In addition to optical properties, self-consistently calculated thermodynamic quantities such as the pressure and internal energy can also be extracted from our model via the standard thermodynamic derivatives of the Helmholtz free energy.

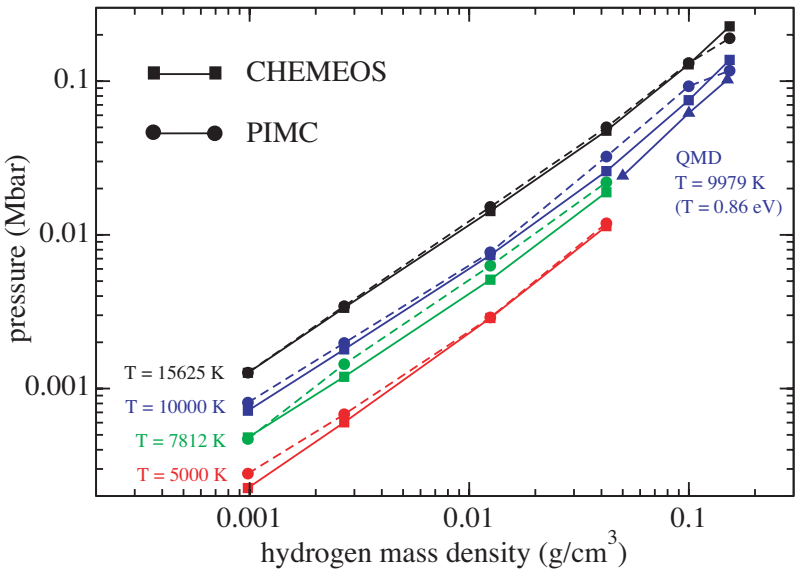

Figure 1—
Comparison of our results for the pressures in hydrogen with path-integral Monte Carlo (PIMC) [6] calculations.

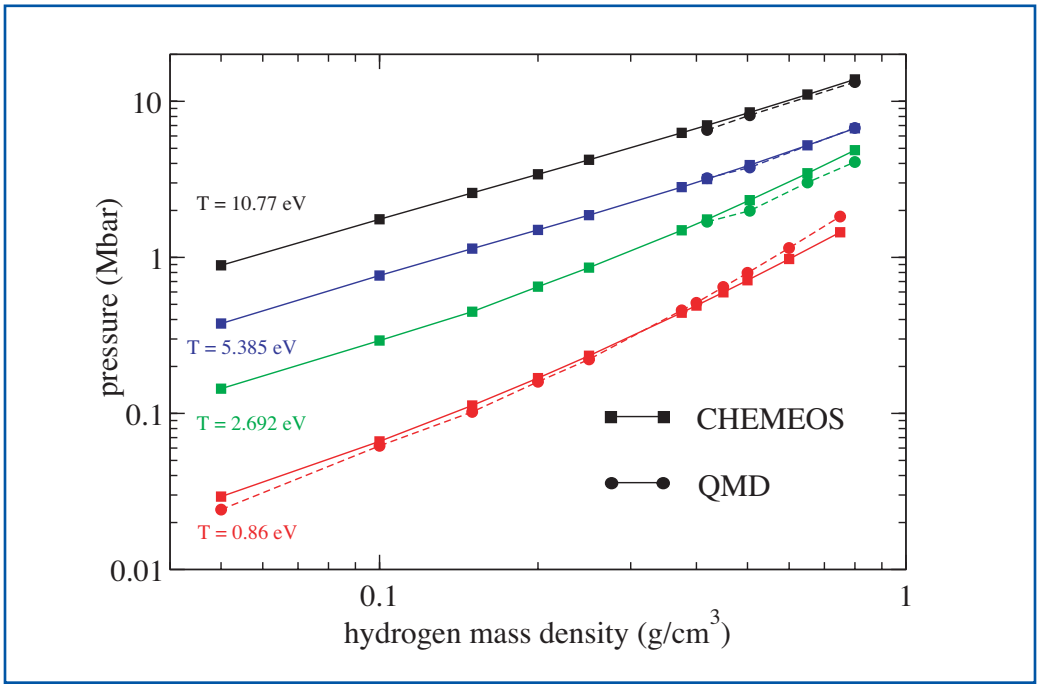

Figure 2—
Comparison of our results for the pressures in hydrogen with quantum molecular dynamics (QMD) [7] calculations.

In Fig. 1 we compare our results for the pressures in hydrogen with path-integral Monte Carlo (PIMC) [6] and in Fig. 2 with quantum molecular dynamics (QMD) [7] calculations. A very good agreement between our chemical model and the two calculations is shown in both cases. We emphasize that in addition to producing results consistent with these sophisticated *ab initio* calculations, our chemical model is also relatively computationally inexpensive and is valid for a wide range of temperature and density parameters. These features make CHEMEOS a good candidate for the generation of the required opacity tables. Work is currently in progress to extend this model to other elements besides hydrogen and to make further comparisons with other models and experimental data.

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